

Methyl 3-butoxypropanoate
4126-55-0 | DTXSID20633950

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 191 °C

Global applicability domain: Inside

Local applicability domain index: 7.38e-01

Confidence level: 8.24e-01

Nearest Neighbors from the Training Set

Image not found

2-Butoxyethyl acetate

Measured: 192

Predicted: 191

Image not found

Butanoic anhydride

Measured: 200

Predicted: 194

Image not found

Diethylene glycol diethyl ether

Measured: 188

Predicted: 183

Image not found

Propane, 1,1,3,3-tetramethoxy-

Measured: 183

Predicted: 177

Image not found

Isobutyric anhydride

Measured: 183

Predicted: 185